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# Digital quantum simulation of quantum dynamics and control

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## Motivation

***Can we use light to control chemistry?***

***Idea***:
Use shaped fields to control molecular systems

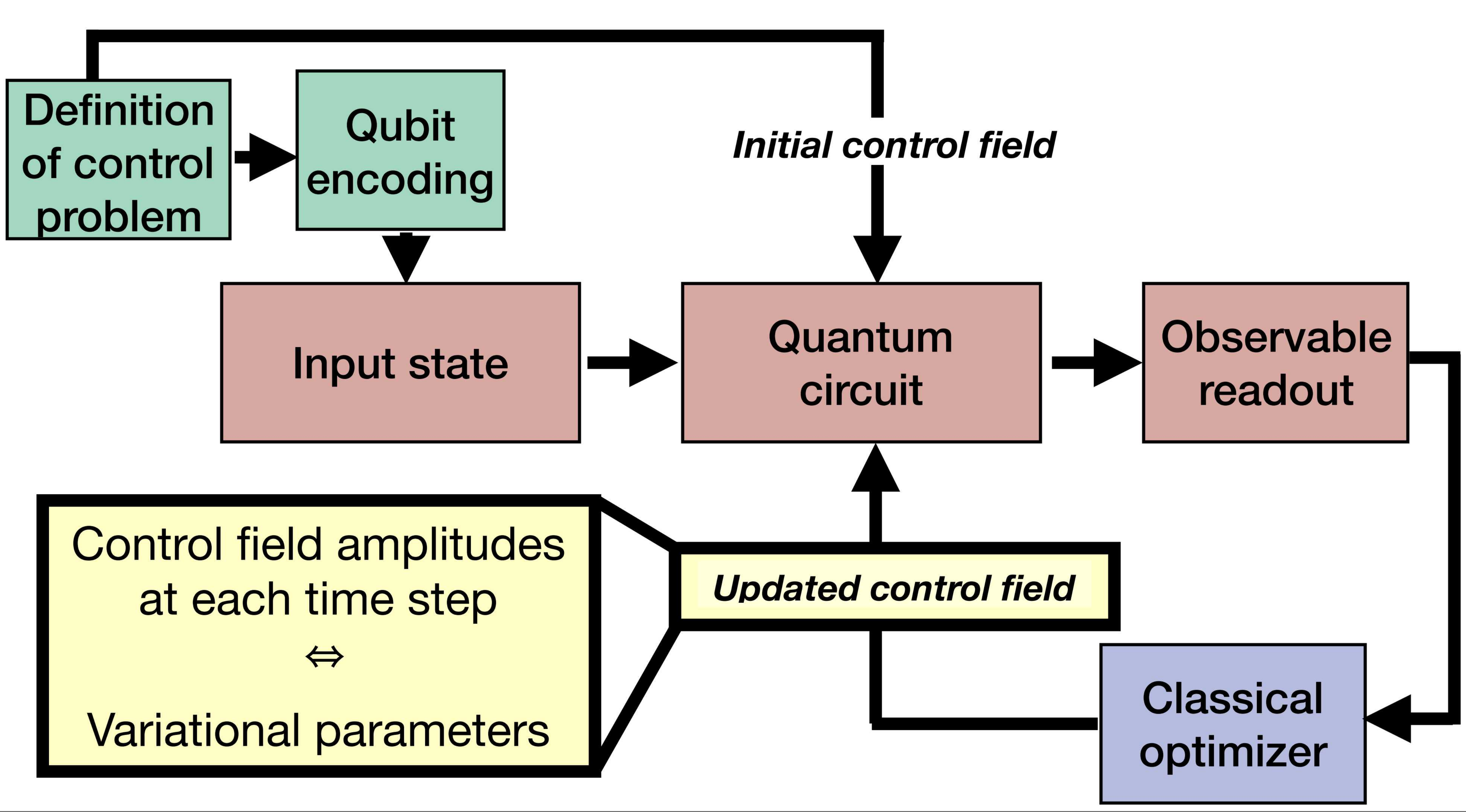
***Challenge***:
Simulations of the dynamics and control of many quantum systems are infeasible

Problem for:
- feasibility studies
- experimental guidance
- control mechanism analysis

**"Curse of dimensionality"**

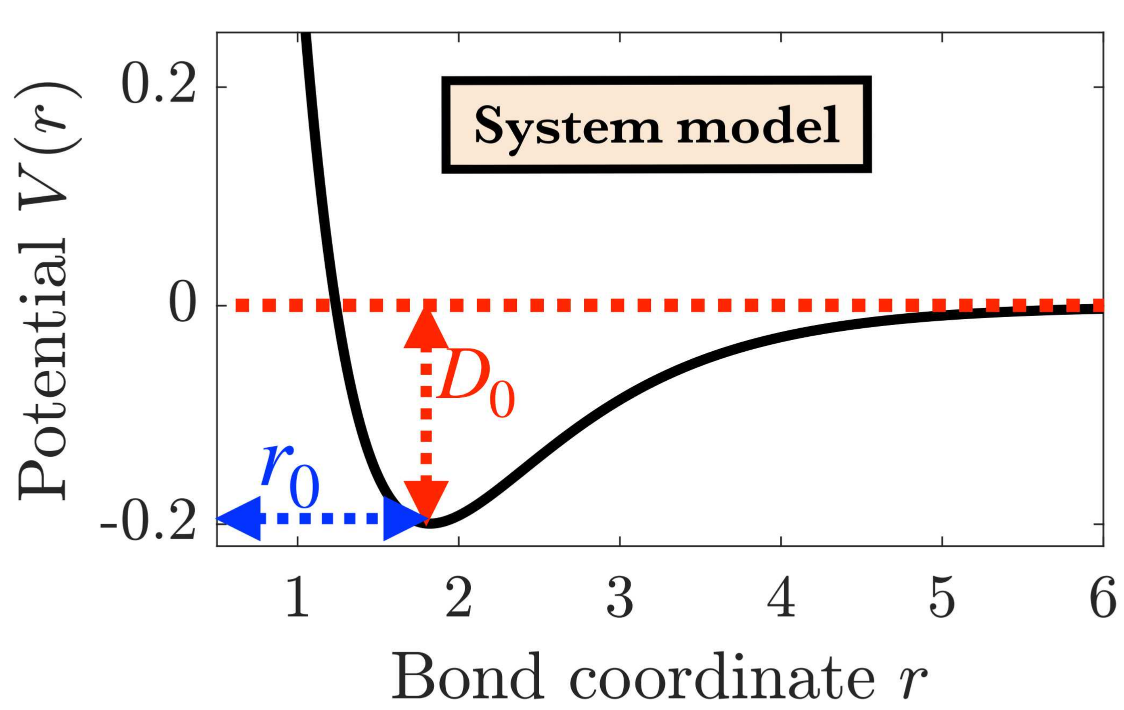
***Goal:***
Explore how a quantum computer could be used to address this challenge by serving as a digital quantum simulator in quantum control simulations

## Simulation framework




## Example problem: Controlling the vibrational state of a molecular bond

**System model**




**Control goal**

Identify field $\varepsilon(t)$ to prepare particular vibrational eigenstate $|v\rangle$ at terminal time T

**Control field specification**

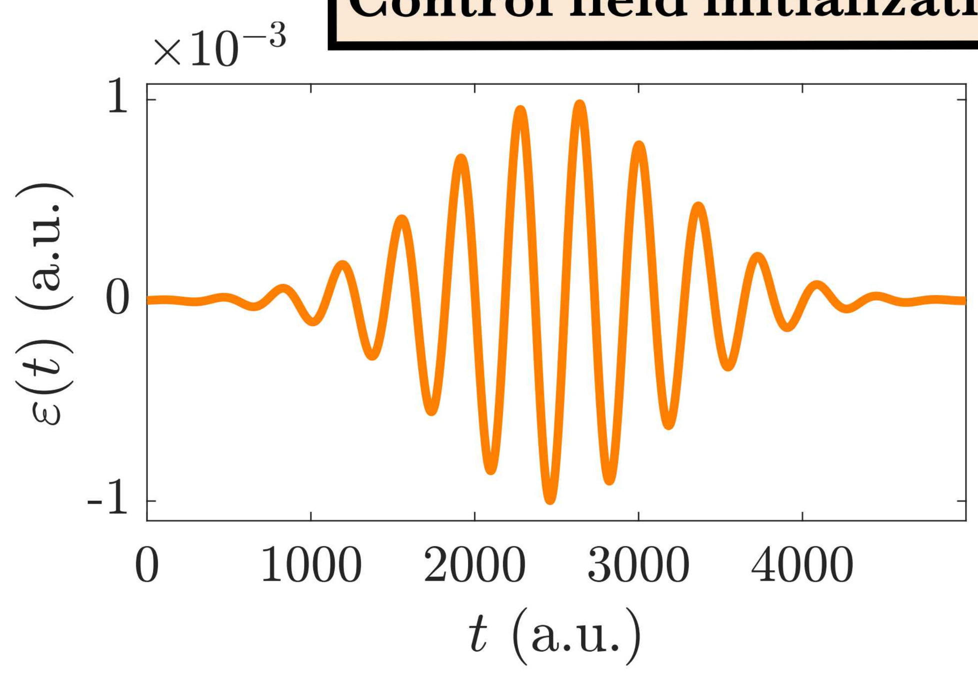
Set pulse duration as

$T = 5{,}000$ **a.u.** $\approx 121$ **fs**

Set time step as

$\Delta t = 2$ **a.u.**

**Control field initialization**




## Illustration

The $k$th vibrational state is encoded as:

$$|k\rangle = |0\rangle_0|0\rangle_1\cdots|0\rangle_{k-1}|1\rangle_k|0\rangle_{k+1}\cdots|0\rangle_{d-1}$$

The operators are encoded as:

$$a^\dagger = \sum_{k=0}^{d-2}\sqrt{k+1}\left(\sigma_-^k\sigma_+^{k+1}\right) \qquad a^\dagger a = \sum_{k=0}^{d-1} k\left(\frac{\sigma_z^k+1}{2}\right)$$

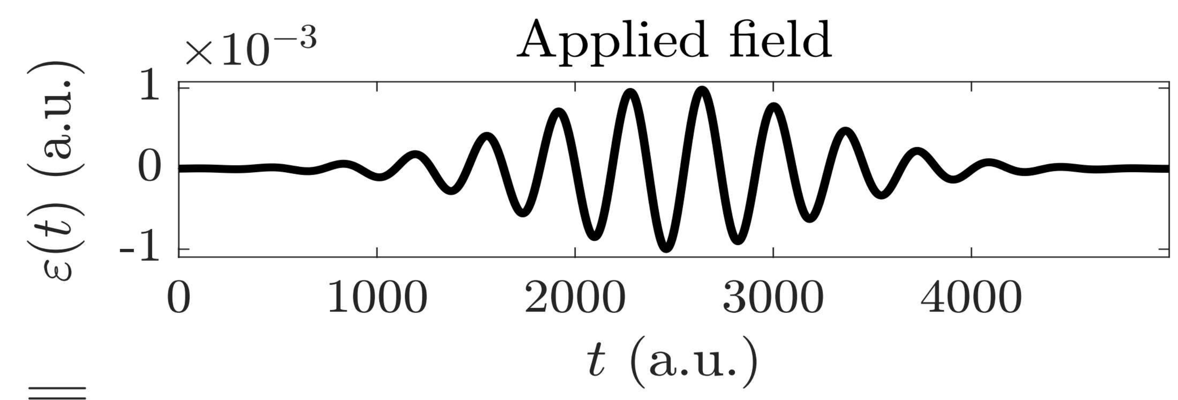
Hamiltonian simulation algorithm used to evolve system under influence of control field

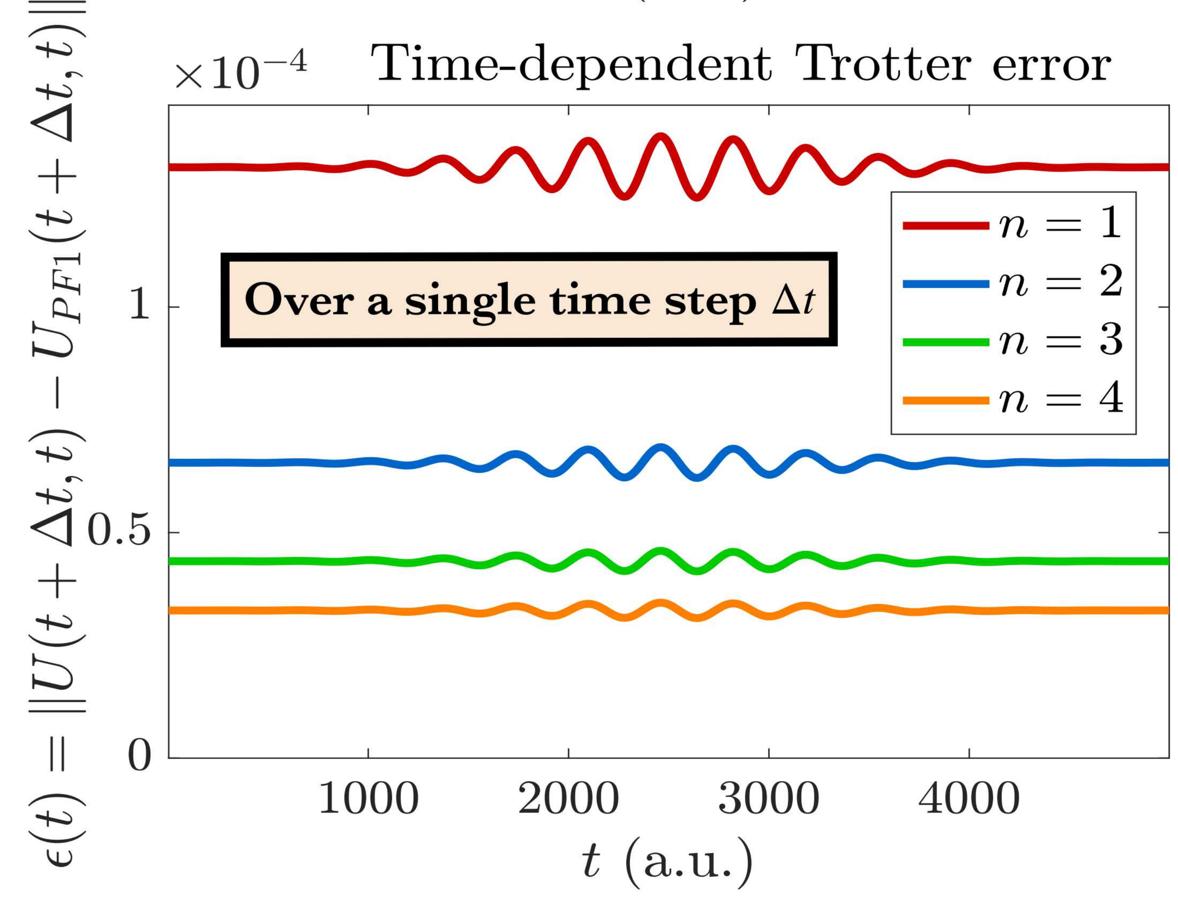
$$e^{-iH(t)\Delta t} \approx \left(e^{-iH_1 t/n}e^{-iH_2 t/n}\cdots e^{-iH_l t/n}\right)^n$$

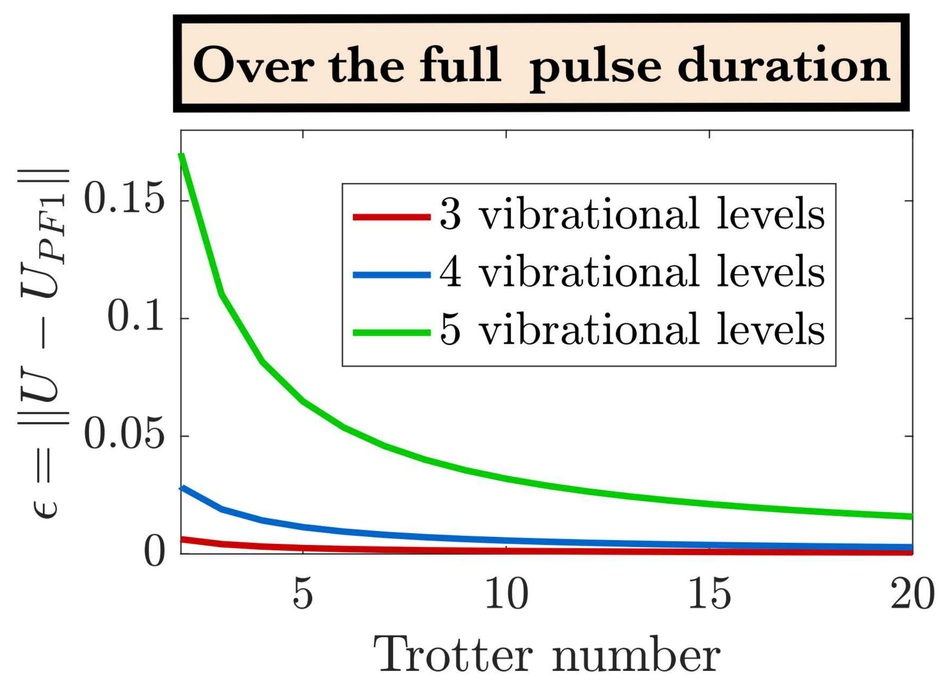
**"Trotter"**

To simulate time evolution over $N$ time steps of length $\Delta t$, take the product

$$e^{-iH(t_N)\Delta t}\cdots e^{-iH(t_1)\Delta t}e^{-iH(t_0)\Delta t}$$




For simulation results, measure qubits in computational basis

## Outlook

- Exploration and comparison of different quantum algorithms for Hamiltonian simulation
- Analysis of the tradeoff between **gradient** and **gradient-free** optimization algorithms for identifying control fields
- Estimation of required quantum resources
- Extensions to quantum control problems with greater complexity

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